

Spiral symmetry and general Bloch's theorem

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1 Abstract

In this paper, spiral symmetry in cylindrical coordinate and general Bloch's theorem induced from it are discussed. This general Bloch's theorem is useful for considering the properties related to single-walled carbon nanotubes.

2 Translation symmetry in \mathbb{R}^3 and Bloch's theorem

Above all, we go over traditional translation symmetry and Bloch's theorem [1].

Lattice vectors:

$$\mathbf{R}_j = n_{j1}\mathbf{a}_1 + n_{j2}\mathbf{a}_2 + n_{j3}\mathbf{a}_3. \quad (1)$$

Hamiltonian:

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r}); \quad V(\mathbf{r} + \mathbf{R}_j) = V(\mathbf{r}). \quad (2)$$

Define translation operators $\mathcal{J}(\mathbf{R}_j)$ ($j \in \mathbb{N}$), which act on a function $f(\mathbf{r})$ as:

$$\mathcal{J}(\mathbf{R}_j)f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}_j). \quad (3)$$

We can easily proof:

$$\mathcal{J}(\mathbf{R}_j)\mathcal{J}(\mathbf{R}_l) = \mathcal{J}(\mathbf{R}_l + \mathbf{R}_j) = \mathcal{J}(\mathbf{R}_j + \mathbf{R}_l) = \mathcal{J}(\mathbf{R}_l)\mathcal{J}(\mathbf{R}_j). \quad (4)$$

Otherwise,

$$\begin{aligned} \mathcal{J}(\mathbf{R}_j)Hf(\mathbf{r}) &= -\frac{\hbar^2}{2\mu}\mathcal{J}(\mathbf{R}_j)\nabla^2 f(\mathbf{r}) + \mathcal{J}(\mathbf{R}_j)V(\mathbf{r})f(\mathbf{r}) \\ &= -\frac{\hbar^2}{2\mu}\nabla^2 \mathcal{J}(\mathbf{R}_j)f(\mathbf{r}) + V(\mathbf{r} + \mathbf{R}_j)f(\mathbf{r} + \mathbf{R}_j) \\ &= [-\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})]f(\mathbf{r} + \mathbf{R}_j) = H\mathcal{J}(\mathbf{R}_j)f(\mathbf{r}). \end{aligned} \quad (5)$$

Therefore $\{\mathcal{J}(\mathbf{R}_j), H\}$ is the set of conserved quantities. In this case, an eigenfunction of the Hamiltonian must be an eigenfunction of the translation operators.

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}) \Rightarrow \mathcal{J}(\mathbf{R}_j)\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R}_j) = \lambda(\mathbf{R}_j)\psi(\mathbf{r}). \quad (6)$$

On the one hand, from Eq.(4), we know

$$\lambda(\mathbf{R}_j)\lambda(\mathbf{R}_l) = \lambda(\mathbf{R}_j + \mathbf{R}_l). \quad (7)$$

On the other hand, the electron density must be periodic, i.e., $|\psi(\mathbf{r} + \mathbf{R}_j)|^2 = |\psi(\mathbf{r})|^2$, from which we know

$$|\lambda(\mathbf{R}_j)|^2 = 1. \quad (8)$$

Eqs(7) and (8) give

$$\lambda(\mathbf{R}_j) = e^{i\boldsymbol{\kappa} \cdot \mathbf{R}_j}. \quad (9)$$

Thus we have Bloch's theorem:

$$\psi(\mathbf{r} + \mathbf{R}_j) = e^{i\boldsymbol{\kappa} \cdot \mathbf{R}_j}\psi(\mathbf{r}). \quad (10)$$

3 Spiral symmetry in cylindrical coordinate and Bloch's theorem

Hamiltonian in cylindrical coordinate:

$$H = -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial \rho^2} + \frac{\partial}{\rho \partial \rho} + \frac{\partial^2}{\rho^2 \partial \theta^2} + \frac{\partial^2}{\partial z^2} \right) + V(\rho, \theta, z), \quad (11)$$

$$V(\rho, \theta, z) = V(\rho, \theta + j_1 \vartheta, z + j_1 \tau + j_2 T), \quad (12)$$

where $\vartheta = 2\pi/N$, $N\tau = MT$, $N, M \in \mathbb{N}$, $j_1, j_2 \in \mathbb{Z}$. Eq.(12) is called the spiral symmetry. Define vectors $\mathbf{r} = (\theta, z)$ and $\mathbf{R}_j = (j_1 \vartheta, j_1 \tau + j_2 T)$ in the space $[0, 2\pi) \times \mathbb{R}$. Define operators $\mathcal{J}(\mathbf{R}_j)$ ($j \in \mathbb{N}$), which act on a function $f(\rho; \mathbf{r})$ as:

$$\mathcal{J}(\mathbf{R}_j)f(\rho; \mathbf{r}) = f(\rho; \mathbf{r} + \mathbf{R}_j). \quad (13)$$

We can easily proof:

$$\mathcal{J}(\mathbf{R}_j)\mathcal{J}(\mathbf{R}_l) = \mathcal{J}(\mathbf{R}_l + \mathbf{R}_j) = \mathcal{J}(\mathbf{R}_j + \mathbf{R}_l) = \mathcal{J}(\mathbf{R}_l)\mathcal{J}(\mathbf{R}_j), \quad (14)$$

and

$$\mathcal{J}(\mathbf{R}_j)V(\rho; \mathbf{r}) = V(\rho; \mathbf{r})\mathcal{J}(\mathbf{R}_j). \quad (15)$$

Otherwise,

$$\mathcal{J}(\mathbf{R}_j) \left(\frac{\partial^2}{\rho^2 \partial \theta^2} + \frac{\partial^2}{\partial z^2} \right) f(\rho; \mathbf{r}) = \left(\frac{\partial^2}{\rho^2 \partial \theta^2} + \frac{\partial^2}{\partial z^2} \right) \mathcal{J}(\mathbf{R}_j) f(\rho; \mathbf{r}). \quad (16)$$

Thus

$$\mathcal{J}(\mathbf{R}_j)H = H\mathcal{J}(\mathbf{R}_j). \quad (17)$$

We can obtain general Bloch's theorem analogizing above section.

$$H\psi(\rho; \mathbf{r}) = E\psi(\rho; \mathbf{r}) \Rightarrow \mathcal{J}(\mathbf{R}_j)\psi(\rho; \mathbf{r}) = \psi(\rho; \mathbf{r} + \mathbf{R}_j) = e^{i\boldsymbol{\kappa} \cdot \mathbf{R}_j} \psi(\rho; \mathbf{r}). \quad (18)$$

We set $\boldsymbol{\alpha}_1 = (\vartheta, \tau)$, $\boldsymbol{\alpha}_2 = (0, T)$, $\boldsymbol{\beta}_1 = (N, 0)$, $\boldsymbol{\beta}_2 = (-\tau N/T, 2\pi/T)$, $\mathbf{G}_j = j_1 \boldsymbol{\beta}_1 + j_2 \boldsymbol{\beta}_2 = (j_1 N - j_2 N \tau/T, 2\pi j_2/T)$, then we can obtain

$$\psi(\rho; \mathbf{r}) = \sum_{\mathbf{j}n} \phi_{n\mathbf{j}}(\rho) e^{i(\boldsymbol{\kappa} + \mathbf{G}_j) \cdot \mathbf{r}} \quad (19)$$

4 Discussion and Potential application

Beginning with Eq.(19), we can continue to construct a method similar to plane wave expansions [2]. We believe general Bloch's theorem will be useful for consider the properties of single-walled carbon nanotubes for their spiral symmetry [3][4].

5 Reference

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